Weakly non-ergodic Statistical Physics

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For weakly non ergodic systems, the probability density function of a time average observable $\overline{\mathcal{O}}$ is $f_\alpha\left(\overline{\mathcal{O}}\right) = -\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}\frac{\sum_{i=1}^{L} p_i^{\mathrm{eq}}(\overline{\mathcal{O}}-\mathcal{O}_i+i\epsilon)^{\alpha-1}}{\sum_{i=1}^{L} p_i^{\mathrm{eq}}(\overline{\mathcal{O}}-\mathcal{O}_i+i\epsilon)^{\alpha}}$ where $\mathcal{O}_i$ is the value of the observable when the system is in state $i = 1, \cdots L$. p_i^{eq} is the probability that a member of an ensemble of systems occupies state i in equilibrium. For a particle undergoing a fractional diffusion process in a binding force field, with thermal detailed balance conditions, p_i^{eq} is Boltzmann's canonical probability. Within the unbiased sub-diffusive continuous time random walk model, the exponent $0 < \alpha < 1$ is the anomalous diffusion exponent $\langle x^2\rangle \sim t^\alpha$ found for free boundary conditions. When $\alpha \to 1$ ergodic statistical mechanics is recovered $\lim_{\alpha\to 1} f_\alpha(\overline{\mathcal{O}}) = \delta\left(\overline{\mathcal{O}} - \langle\mathcal{O}\rangle\right)$. We briefly discuss possible physical applications in single particle experiments.

I. INTRODUCTION

An ensemble of non-interacting one dimensional Brownian particles in the presence of a binding potential field $V(x)$ reach a thermal equilibrium described by Boltzmann's canonical law $p^{\mathrm{eq}}(x) = \exp[-V(x)/T]/Z$ where T is the temperature (units $k_b = 1$) and Z is the normalizing partition function. With this law we may calculate ensemble averages for example $\langle x\rangle = \int_{-\infty}^{\infty} x p^{\mathrm{eq}}(x)\mathrm{d}x$. On the other hand from the trajectory of a single particle $x(t)$ we may construct the time average $\overline{x} = \int_0^t x(t')\mathrm{d}t'/t$. For ergodic motion the time and ensemble averages are identical in the limit of long measurement times $t \to \infty$. What is the Physical meaning of a long measurement time? Brownian dynamics in a finite interval, is characterized by a finite relaxation time which is the time scale on which particles reach thermal equilibrium. For the simplest case of Brownian motion between two reflecting walls, with a system of size l, dimensional analysis gives a relaxation time of the order l^2/D where D is the diffusion constant. A second time scale, the average time between jump events $\langle\tau\rangle$ is more microscopical. The latter is related to D with the Einstein relation [1] $D = \langle(\Delta x)^2\rangle/2\langle\tau\rangle$ where $\langle(\Delta x)^2\rangle$ is the variance of jump lengths. Ergodicity is almost trivial when the measurement time is much longer than these two time scales. For example for a Brownian motion in a Harmonic field.

On the other hand anomalous diffusion and transport, is characterized in many cases by a diverging relaxation time and a diverging microscopical time scale $\langle\tau\rangle$. For example unbiased sub-diffusion is characterized by a mean square displacement $\langle x^2\rangle \propto t^\alpha$ and $0 < \alpha < 1$. The reader immediately realizes that the diffusion constant is zero, in the sense that $\lim_{t\to\infty}\langle x^2\rangle/t = 0$, hence the mentioned relaxation time l^2/D is infinite even when the system size l is finite. Indeed according to the continuous time random walk (CTRW) model [2, 3, 4, 5, 6], anomalous sub-diffusion is found when waiting times between jumps diverge $\langle\tau\rangle \to \infty$, which is related to the Scher-Montroll power law waiting time probability density function (PDF) $\psi(\tau) \propto \tau^{-(1+\alpha)}$ [2]. For such scale free anomalous diffusion the relaxation time and the averaged sojourn time $\langle\tau\rangle$ are infinite, and ergodicity is broken weakly.

Strong ergodicity breaking is found when a system is divided into inaccessible regions of its phase space. Namely a particle or a system starting in one region cannot explore all other regions due to some non-passable barrier (e.g. in the micro-canonical case, by regions we mean sections on the constant energy surface). Bouchaud [7] introduced the profound concept of weak ergodicity breaking in the context of glass dynamics, which in turn is related to infinite ergodic theory [8] investigated by Mathematicians using a dynamical approach. In weak ergodicity breaking the phase space is not broken into inaccessible regions. Instead due to the power law sticking times the dynamics is non-stationary and non-ergodic. Since the ergodic hypothesis is the pillar on which statistical mechanics is built, but at the same time also long tailed power law distributions of trapping times are very common in the description of Physical behaviors [2, 3, 4, 5, 6], it is natural to investigate the non-ergodic properties of systems whose stochastic dynamics are governed by such anomalous statistics. Previously weak ergodicity breaking was investigated for: blinking quantum dots [9, 10, 11, 12], Lévy walks [13] occupation time statistics of the CTRW model [14, 15], fractional Fokker-Planck equation [16], deterministic one dimensional maps [17, 18, 19], numerical simulations of fractional transport in a washboard potential [20] and in vivo gene regulation by DNA-binding proteins [21]. Recently a relation between statistics of weak ergodicity breaking and statistics of non-self averaging in models of quenched disorder was found [22]. Hence it is timely to present a general statistical mechanical framework for weak-ergodicity breaking.

In this manuscript we investigate the distribution of time averaged observables for weak ergodicity breaking. We explore the relations between ensemble averages and fluctuations of time averages. And investigate the transition from the localization limit $\alpha \to 0$ to the usual

ergodic behavior found for $\alpha \to 1$. Specific examples for the distribution of $\overline{x}$ for a particle undergoing a subdiffusive CTRW in a potential $V(x)$ are worked out is detail. In the second part of the paper we derive our main results using a generalized CTRW approach. We investigate models with a single waiting time PDF and more general models with several types of such PDFs. A brief summary of some of our results was recently published in [23].

The theory of weak-ergodicity breaking is mathematically related to the arcsine distribution [24, 25, 26], and to its extensions [27, 28]. Consider a normal Brownian motion with free boundary conditions in one dimension $\dot{x}(t) = \eta(t)$ where $\eta(t)$ is Gaussian white noise. The time t^+ spent by the particle in $x > 0$ is called an occupation time. Naive expectation is that the single particle will occupy $x > 0$ for half of the measurement time t, when the latter is long. Instead the PDF of the occupation fraction is

$$f\left(\frac{t^+}{t}\right) = \frac{1}{\pi\sqrt{(t^+/t)\left(1 - t^+/t\right)}}. \quad (1)$$

This arcsine law is related to the well known PDF of first-passage times from x to the origin, for simple Brownian motion. The latter PDF decays $t^{-3/2}$ for long first-passage times [25], and the averaged return time is infinite. Roughly speaking, during the dynamics of the particle, it will usually occupy either the domain $x > 0$ or the domain $x < 0$ for a duration which is of the order of the measurement time. Thus the arcsine PDF Eq. (1) has a U shape. This behavior is found because the Brownian motion was assumed to be unbounded. If we add reflecting walls on $x = l/2$ and $x = -l/2$ the dynamics will be ergodic and in the long time limit the particle spends half of the time in $(0, l/2)$ and the other half in $(-l/2, 0)$. The theory of weak ergodicity breaking, presented in this manuscript, is mathematically related to the arcsine law and is based on Lévy statistics.

This paper is organized as follows. In Sec. II distribution of time averaged observables for weakly non-ergodic systems is presented using general arguments not specific to a model. Properties of this distribution are investigated in Sec. III and in Sec. IV the example of the distribution of $\overline{x}$ for a particle undergoing fractional dynamics in a binding potential is worked out in detail. In Sec. V we derive our main result using a CTRW approach, thus further justifying assumptions made in Sec. II. Numerical simulations of $\overline{x}$ obtained from the CTRW

process are compared with analytical theory in sub-Sec. V A.

II. DISTRIBUTION OF TIME AVERAGED OBSERVABLES

We consider a system with L states and label them with an index $i = 1, ...L$. A time average of a Physical observable $\mathcal{O}$ is made. If the system is in state i the Physical observable attains the value $\mathcal{O}_i$. The time the system spends in state i is t_i and is called a residence time or an occupation time. The time average of the Physical observable is

$$\overline{\mathcal{O}} = \frac{\sum_{i=1}^{L} t_i \mathcal{O}_i}{\sum_{i=1}^{L} t_i} \quad (2)$$

and $\min\{\mathcal{O}_i\} \leq \overline{\mathcal{O}} \leq \max\{\mathcal{O}_i\}$. As mentioned in the introduction many physical systems, in their stochastic or deterministic dynamics, are known to be characterized by power law sojourn times in the states of the system [2, 3, 4, 5, 6]. We assume that the occupation time t_i is a sum of many such sojourn times. If the state i is visited many times, and the sojourn times are independent identically distributed random variables, Lévy's limit theorem will describe the statistics of the residence times t_i in the limit of long measurement time. Hence we argue that the PDF of t_i is a one sided Lévy PDF $l_{\alpha, p_i^{\text{eq}}}(t_i)$ whose Laplace transform is

$$\int_0^\infty l_{\alpha, p_i^{\text{eq}}}(t_i) \exp(-ut_i)\mathrm{d}t_i = \exp\left(-p_i^{\text{eq}} u^\alpha\right) \quad (3)$$

and $0 < \alpha \leq 1$ [29]. Later we find that p_i^{eq} is the probability that a member of an ensemble of systems occupies state i in equilibrium. For the CTRW with thermal detailed balance conditions p_i^{eq} is Boltzmann's probability of finding the system in state i, $p_i^{\text{eq}} = \exp(-E_i/T)/Z$ as we will show later.

The following generating function [26] is a useful tool

$$\hat{f}_\alpha(\xi) = \langle \frac{1}{1 + \xi\overline{\mathcal{O}}} \rangle = \sum_{k=0}^{\infty} (-1)^k \langle \overline{\mathcal{O}}^k \rangle \xi^k. \quad (4)$$

Our main aim is to find the PDF of the time averaged observable

$$f_\alpha\left(\overline{\mathcal{O}}\right) = \langle \delta\left(\overline{\mathcal{O}} - \frac{\sum_{i=1}^{L} \mathcal{O}_i t_i}{\sum_{i=1}^{L} t_i}\right) \rangle = -\frac{1}{\pi}\lim_{\epsilon \to 0}\text{Im}\langle \frac{1}{\overline{\mathcal{O}} + i\epsilon - \frac{\sum_{i=1}^{L} \mathcal{O}_i t_i}{\sum_{i=1}^{L} t_i}} \rangle = -\frac{1}{\pi}\lim_{\epsilon \to 0}\text{Im}\frac{1}{\overline{\mathcal{O}} + i\epsilon}\langle \frac{1}{1 - \frac{1}{\overline{\mathcal{O}} + i\epsilon}\frac{\sum_{i=1}^{L} \mathcal{O}_i t_i}{\sum_{i=1}^{L} t_i}} \rangle, \quad (5)$$

using Eq. (4)

$$f_\alpha\left(\overline{\mathcal{O}}\right) = -\frac{1}{\pi}\lim_{\epsilon\to 0}\text{Im}\frac{1}{\overline{\mathcal{O}}+i\epsilon}\hat{f}_\alpha\left(-\frac{1}{\overline{\mathcal{O}}+i\epsilon}\right) \qquad (6)$$

We now find the generating function Eq. (4) and invert it using Eq. (6) to obtain $f_\alpha\left(\overline{\mathcal{O}}\right)$.

The generating function is rewritten

$$\hat{f}_\alpha\left(\xi\right) = \langle\int_0^\infty \mathrm{d}s e^{-\left(1+\xi\frac{\sum_{i=1}^L \mathcal{O}_i t_i}{\sum_{i=1}^L t_i}\right)s}\rangle =$$

$$\int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}t \int_0^\infty \mathrm{d}t_1 l_{\alpha,p_1^{\text{eq}}}(t_1)\cdots\int_0^\infty \mathrm{d}t_L l_{\alpha,p_L^{\text{eq}}}(t_L)\delta\left(t-\sum_{i=1}^L t_i\right)e^{-\left(1+\xi\frac{\sum_{i=1}^L \mathcal{O}_i t_i}{t}\right)s}. \qquad (7)$$

Using a well known presentation for the delta function in Eq. (7)

$$\delta\left(t-\sum_{i=1}^L t_i\right) = \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}k e^{ik\left(t-\sum_{i=1}^L t_i\right)}, \qquad (8)$$

changing variables $kt = \tilde{k}$ and using Eq. (3) we find

$$\hat{f}_\alpha\left(\xi\right) = \int_0^\infty \mathrm{d}t t^{-1}\int_{-\infty}^\infty \frac{\mathrm{d}\tilde{k}}{2\pi}\int_0^\infty \mathrm{d}s \exp\left[i\tilde{k}-s-\sum_{i=1}^L p_i^{\text{eq}}\frac{\left(i\tilde{k}+\mathcal{O}_i\xi s\right)^\alpha}{t^\alpha}\right]. \qquad (9)$$

We again change variables $k = \tilde{k}/t$ and $\tilde{s} = s/t$ and obtain

$$\hat{f}_\alpha\left(\xi\right) = \int_0^\infty \mathrm{d}t\int_{-\infty}^\infty \frac{\mathrm{d}k}{2\pi}\int_0^\infty \mathrm{d}\tilde{s} t \exp\left[ikt-\tilde{s}t-\sum_{i=1}^L p_i^{\text{eq}}\left(ik+\mathcal{O}_i\xi\tilde{s}\right)^\alpha\right]. \qquad (10)$$

This equation is rewritten using a simple trick

$$\hat{f}_\alpha\left(\xi\right) = \int_0^\infty \mathrm{d}t\int_\infty^\infty \frac{\mathrm{d}k}{2\pi}\int_0^\infty \mathrm{d}\tilde{s}\left\{-\frac{\mathrm{d}}{\mathrm{d}\tilde{s}}\exp\left[ikt-\tilde{s}t-\sum_{i=1}^L p_i^{\text{eq}}\left(ik+\mathcal{O}_i\xi\tilde{s}\right)^\alpha\right]\right.$$

$$\left.-\alpha\sum_{i=1}^L p_i^{\text{eq}}\left(ik+\mathcal{O}_i\xi\tilde{s}\right)^{\alpha-1}\mathcal{O}_i\xi \exp\left[\left(ik-\tilde{s}\right)t-\sum_{i=1}^L p_i^{\text{eq}}\left(ik+\mathcal{O}_i\xi\tilde{s}\right)^\alpha\right]\right\}. \qquad (11)$$

Integration over t gives a simple pole $1/(ik-\tilde{s})$, using Cauchy integral formula to integrate over k, and then solving two trivial integrals yields

$$\hat{f}_\alpha\left(\xi\right) = \frac{\sum_{i=1}^L p_i^{\text{eq}}\left(1+\mathcal{O}_i\xi\right)^{\alpha-1}}{\sum_{i=1}^L p_i^{\text{eq}}\left(1+\mathcal{O}_i\xi\right)^\alpha}. \qquad (12)$$

Inverting Eq. (12) using Eq. (6) we find

$$f_\alpha\left(\overline{\mathcal{O}}\right) = -\frac{1}{\pi}\lim_{\epsilon\to 0}\text{Im}\frac{\sum_{i=1}^L p_i^{\text{eq}}\left(\overline{\mathcal{O}}-\mathcal{O}_i+i\epsilon\right)^{\alpha-1}}{\sum_{i=1}^L p_i^{\text{eq}}\left(\overline{\mathcal{O}}-\mathcal{O}_i+i\epsilon\right)^\alpha}. \qquad (13)$$

This is a very general formula for the distribution of time averaged observables for weakly non-ergodic systems. As we show later, within the CTRW model, α is the anomalous diffusion exponent. For $0 < \alpha < 1$ we use $\lim_{\epsilon\to 0}\left(\overline{\mathcal{O}}-\mathcal{O}_i+i\epsilon\right)^\alpha = |\overline{\mathcal{O}}-\mathcal{O}_i|^\alpha e^{i\phi_i\alpha}$ where

$$\phi_i = \left(\begin{array}{c}\pi \text{ if } \overline{\mathcal{O}} < \mathcal{O}_i \\ 0 \text{ if } \overline{\mathcal{O}} \geq \mathcal{O}_i\end{array}\right) \text{ and Eq.(13) becomes}$$

$$f_\alpha\left(\overline{\mathcal{O}}\right) =$$

$$\frac{\sin \pi\alpha}{\pi} \frac{I_{\alpha-1}^< \left(\overline{\mathcal{O}}\right) I_{\alpha}^\geq \left(\overline{\mathcal{O}}\right) + I_{\alpha-1}^\geq \left(\overline{\mathcal{O}}\right) I_{\alpha}^< \left(\overline{\mathcal{O}}\right)}{\left[I_{\alpha}^\geq \left(\overline{\mathcal{O}}\right)\right]^2 + \left[I_{\alpha}^< \left(\overline{\mathcal{O}}\right)\right]^2 + 2 I_{\alpha}^\geq \left(\overline{\mathcal{O}}\right) I_{\alpha}^< \left(\overline{\mathcal{O}}\right) \cos \pi\alpha}, \tag{14}$$

with

$$I_\alpha^< \left(\overline{\mathcal{O}}\right) = \sum_{\overline{\mathcal{O}} < \mathcal{O}_i} p_i^{\mathrm{eq}} |\overline{\mathcal{O}} - \mathcal{O}_i|^\alpha \tag{15}$$

and

$$I_\alpha^\geq \left(\overline{\mathcal{O}}\right) = \sum_{\overline{\mathcal{O}} \geq \mathcal{O}_i} p_i^{\mathrm{eq}} |\overline{\mathcal{O}} - \mathcal{O}_i|^\alpha. \tag{16}$$

Notice the L divergences of $f_\alpha(\overline{\mathcal{O}})$ when $\overline{\mathcal{O}} = \mathcal{O}_i$ due to the $I_{\alpha-1}^\geq(\mathcal{O})$ term in the numerator of Eq. (14). This behavior is caused by long sticking times in a state of the system, on a time scale which is of the order of the measurement time.

III. STATISTICS OF WEAK ERGODICITY BREAKING

In this Sec. we investigate properties of Eqs. (12,13).

A. Limits $\alpha \to 0$ and $\alpha \to 1$

In the limit $\alpha \to 1$ we recover usual ergodic behavior. From Eq. (13)

$$f_1 \left(\overline{\mathcal{O}}\right) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \mathrm{Im} \frac{\sum_{i=1}^L p_i^{\mathrm{eq}}}{\sum_{i=1}^L p_i^{\mathrm{eq}} \left(\overline{\mathcal{O}} - \mathcal{O}_i + i\epsilon\right)}. \tag{17}$$

Using the normalization condition $\sum_{i=1}^L p_i^{\mathrm{eq}} = 1$ and the ensemble average

$$\langle \mathcal{O} \rangle = \sum_{i=1}^L p_i^{\mathrm{eq}} \mathcal{O}_i \tag{18}$$

we have ergodic behavior

$$f_1 \left(\overline{\mathcal{O}}\right) = \delta(\overline{\mathcal{O}} - \langle \mathcal{O} \rangle) \tag{19}$$

in the sense that the ensemble average is equal to the time average. Note that already Eq. (3) in the limit $\alpha \to 1$ indicates ergodicity since the residence time is not a fluctuating quantity (i.e. the one sided Lévy PDF is a delta function when $\alpha = 1$). In the opposite limit of $\alpha \to 0$ we find

$$\lim_{\alpha \to 0} f_\alpha \left(\overline{\mathcal{O}}\right) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \mathrm{Im} \sum_{i=1}^L p_i^{\mathrm{eq}} \left(\overline{\mathcal{O}} - \mathcal{O}_i + i\epsilon\right)^{-1} \tag{20}$$

hence

$$\lim_{\alpha \to 0} f_\alpha \left(\overline{\mathcal{O}}\right) = \sum_{i=1}^L p_i^{\mathrm{eq}} \delta \left(\overline{\mathcal{O}} - \mathcal{O}_i\right). \tag{21}$$

This describes a localization behavior where the system is stuck in one of the states for the whole duration of the observation time, which is the expected behavior when $\alpha \to 0$.

B. Lamperti Statistics of the Occupation fraction

Let the Physical observable be $\mathcal{O}_i = 1$ when $i = 1, ..., \bar{l}$ where $\bar{l} \leq L$, otherwise $\mathcal{O}_i = 0$. Hence the time average in this case is the occupation fraction

$$\overline{\mathcal{O}} = \frac{\sum_{i=1}^{\bar{l}} t_i}{\sum_{i=1}^L t_i} \tag{22}$$

which is the fraction of time spent by the system in the observation domain $i = 1, \cdots, \bar{l}$. Clearly $0 \leq \overline{\mathcal{O}} \leq 1$ in this case. Using Eq. (13) a straight forward calculation gives

$$f_\alpha \left(\overline{\mathcal{O}}\right) = \frac{1}{\pi} \frac{\mathcal{R} \left[\left(1 - \overline{\mathcal{O}}\right) \overline{\mathcal{O}}\right]^{\alpha-1} \sin \pi\alpha}{\mathcal{R}^2 \left(1 - \overline{\mathcal{O}}\right)^{2\alpha} + \overline{\mathcal{O}}^{2\alpha} + 2\mathcal{R} \left[\left(1 - \overline{\mathcal{O}}\right) \overline{\mathcal{O}}\right]^\alpha \cos \pi\alpha}. \tag{23}$$

This is the Lamperti PDF [27] which is a natural generalization of the arcsine distribution [the case $\alpha = 1/2, \mathcal{R} = 1$ Eq. (1)]. The PDF Eq. (23) has found several applications in non-ergodic systems mentioned in the introduction [10, 14, 17, 18, 19, 21] and recently for the non-self averaging properties of the quenched trap model [22]. The parameter $\mathcal{R}$ in Eq. (23) is called the asymmetry parameter and is given by

$$\mathcal{R} = \frac{p_{1,\bar{l}}^{\mathrm{eq}}}{1 - p_{1,\bar{l}}^{\mathrm{eq}}} \tag{24}$$

where $p_{1,\bar{l}}^{\mathrm{eq}} = \sum_{i=1}^{\bar{l}} p_i^{\mathrm{eq}}$ is the probability in ensemble sense to be in the observation domain. Since the observable attains two values $\mathcal{O}_i = 1$ or $\mathcal{O}_i = 0$ the PDF Eq. (23) has two divergences on $\overline{\mathcal{O}} = 1$ and $\overline{\mathcal{O}} = 0$ which is a special case of the more general rule discussed after Eq. (16).

C. Low order moments of time averaged observables

From the moment generating function $\hat{f}_\alpha(\xi)$ we can obtain moments of the time averages $\overline{\mathcal{O}}$

$$\langle \overline{\mathcal{O}}^n \rangle = (-1)^n \frac{1}{n!} \frac{\partial^n}{\partial \xi^n} \hat{f}_\alpha \left(\xi\right)|_{\xi=0}. \tag{25}$$

Using Eq. (12) we find

$$\langle \overline{\mathcal{O}} \rangle = \sum_{i=1}^L p_i^{\mathrm{eq}} \mathcal{O}_i. \tag{26}$$

The average $\langle....\rangle$ is over an ensemble of realizations. If the ensemble reaches an equilibrium then obviously $\langle\overline{\mathcal{O}}\rangle = \langle\mathcal{O}\rangle$ which is time independent. Hence the p_i^{eq}s in Eq. (26) are the probabilities that a member of an ensemble of systems occupies state i when the ensemble reaches an equilibrium. This justifies our original assumption that the p_i^{eq}s in Eq. (3) are population fractions. Namely the p_i^{eq}s can be in principle measured by letting many independent systems (or many non-interacting particles) evolve and then in the long time limit p_i^{eq} is the number of systems in state i over the total number of systems when the latter is large. Using Eqs. (12,25) the fluctuations are given by

$$\langle\overline{\mathcal{O}^2}\rangle - \langle\overline{\mathcal{O}}\rangle^2 = (1-\alpha)\left(\langle\mathcal{O}^2\rangle - \langle\mathcal{O}\rangle^2\right) \qquad (27)$$

where $\langle\mathcal{O}^2\rangle = \sum_{i=1}^L p_i^{\text{eq}}(\mathcal{O}_i)^2$. Eq. (27) gives a simple relation between fluctuations of time averages and fluctuations of ensemble averages. Once again when $\alpha = 1$ the fluctuations of the time average Eq. (27) vanish, indicating ergodic behavior. Relations between cumulants of time average observables and cumulants of ensemble averages are found in a similar way. For the third cumulant

$$C_3(\bar{\mathcal{O}}) = \langle\bar{\mathcal{O}}^3\rangle - 3\langle\bar{\mathcal{O}}^2\rangle\langle\bar{\mathcal{O}}\rangle + 2\langle\bar{\mathcal{O}}\rangle^3 = \frac{1}{2}(2-\alpha)(1-\alpha)\left(\langle\mathcal{O}^3\rangle - 3\langle\mathcal{O}^2\rangle\langle\mathcal{O}\rangle + 2\langle\mathcal{O}\rangle^3\right) = \frac{1}{2}(2-\alpha)(1-\alpha)C_3(\mathcal{O}) \quad (28)$$

and the fourth cumulant

$$C_4(\bar{\mathcal{O}}) = \langle\bar{\mathcal{O}}^4\rangle - 4\langle\bar{\mathcal{O}}^3\rangle\langle\bar{\mathcal{O}}\rangle - 3\langle\bar{\mathcal{O}}^2\rangle^2 + 12\langle\bar{\mathcal{O}}^2\rangle\langle\bar{\mathcal{O}}\rangle^2 - 6\langle\bar{\mathcal{O}}\rangle^4 =$$

$$(1-\alpha)\left(\frac{(3-\alpha)(2-\alpha)}{6}\left(\langle\mathcal{O}^4\rangle - 4\langle\mathcal{O}^3\rangle\langle\mathcal{O}\rangle\right) + \left(6-6\alpha+\alpha^2\right)\left(\langle\mathcal{O}\rangle^2\left(2\langle\mathcal{O}^2\rangle - \langle\mathcal{O}\rangle^2\right)\right) - \frac{1}{2}(6-\alpha)(1-\alpha)\langle\mathcal{O}^2\rangle^2\right).$$

$$(29)$$

Low order moments of time averaged observables can be expressed using the cumulants Eqs. (27,28,29) the results remain as cumbersome as the expressions in Eqs. (28,29). When the odd moments of the ensemble average are equal zero $\langle\mathcal{O}^{2n-1}\rangle = 0$ $n = 1, 2, \cdots$, corresponding to examples we investigate in Sec. IV, the expressions for moments are simpler. Odd moments of the time average observable are equal zero, as expected. The second moment is $\langle\overline{\mathcal{O}}^2\rangle = (1-\alpha)\langle\mathcal{O}^2\rangle$ and the fourth moment

$$\langle\overline{\mathcal{O}}^4\rangle = \frac{(3-\alpha)(2-\alpha)(1-\alpha)}{6}\langle\mathcal{O}^4\rangle + \frac{\alpha(1-\alpha)^2}{2}\langle\mathcal{O}^2\rangle^2. \qquad (30)$$

D. Correlations Between Occupation Fractions $\langle\overline{p}_l\overline{p}_k\rangle$

The correlations between the occupation fractions $\overline{p}_l = t_l/t$ and $\overline{p}_k = t_k/t$ where $t = \sum_{i=1}^L t_i$ are now briefly investigated. We use the L dimensional vector $\vec{\xi} = \{\xi_1, \xi_2, \cdots \xi_L\}$ and the L dimensional generating function

$$\hat{g}_\alpha\left(\vec{\xi}\right) = \langle\frac{1}{1 + \sum_{i=1}^L \xi_i \overline{p}_i}\rangle. \qquad (31)$$

Related multidimensional arcsine distribution of occupation fractions were investigated in [28]. Using the sub-

stitution $\xi\mathcal{O}_i \to \xi_i$ in Eq. (4) it is easy to see using Eq. (12)

$$\hat{g}_\alpha\left(\vec{\xi}\right) = \frac{\sum_{i=1}^L p_i^{\text{eq}}(1+\xi_i)^{\alpha-1}}{\sum_{i=1}^L p_i^{\text{eq}}(1+\xi_i)^\alpha}. \qquad (32)$$

This multidimensional generating function yields

$$\langle\overline{p}_i\rangle = -\frac{\partial}{\partial\xi_i}\hat{g}_\alpha\left(\vec{\xi}\right)|_{\vec{\xi}=0} = p_i^{\text{eq}} \qquad (33)$$

and similarly by taking the second order derivative of $\hat{g}_\alpha(\vec{\xi})$ with respect to ξ_i

$$\langle\overline{p}_i^2\rangle - \langle\overline{p}_i\rangle^2 = (1-\alpha)\,p_i^{\text{eq}}\left(1 - p_i^{\text{eq}}\right). \qquad (34)$$

Identical results can be obtained using the Lamperti PDF Eq. (23). More interesting is to notice the correlations between occupation fractions for example

$$\langle\overline{p}_l\overline{p}_k\rangle = \frac{1}{2}\frac{\partial}{\partial\xi_k}\frac{\partial}{\partial\xi_l}\hat{g}_\alpha\left(\vec{\xi}\right)|_{\vec{\xi}=0} \qquad (35)$$

for $l \neq k$. Using Eq. (32)

$$\langle\overline{p}_l\overline{p}_k\rangle = \alpha p_l^{\text{eq}} p_k^{\text{eq}}. \qquad (36)$$

We see that when $\alpha \to 1$ the occupation fractions are uncorrelated since $\langle\overline{p}_l\overline{p}_k\rangle - \langle\overline{p}_l\rangle\langle\overline{p}_k\rangle = 0$ and one can show

that they are independent random variables. When $\alpha \to 0$ the system occupies one state for practically the whole duration of the measurement hence either $\overline{p}_l \simeq 1$ and then obviously $\overline{p}_k \simeq 0$ or the opposite situation is found, or both occupation fractions are zero (if $L > 2$). In any case clearly the product $\overline{p}_l \overline{p}_k$ is zero when $\alpha \to 0$ and $l \neq k$ as we have indeed found in Eq. (36).

IV. DISTRIBUTION OF $\overline{x}$

We now consider a particle undergoing stochastic fractional dynamics in a binding field. The fractional Fokker–Planck equation [32, 33] describes anomalous sub-diffusion and relaxation close to thermal equilibrium using fractional calculus

$$\frac{\partial^\alpha p(x,t)}{\partial t^\alpha} = D_\alpha \left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{T} \right] p(x,t) \qquad (37)$$

where D_α is the fractional diffusion coefficient, and $F(x) = -\partial V(x)/\partial x$ is the force. Eq. (37) reduces to the usual Fokker-Planck equation when $\alpha = 1$. The fractional Fokker-Planck equation was derived from the sub-diffusive continuous time random walk [33] which is the stochastic process we have in mind. In the absence of the force field and for free boundary conditions $\langle x^2 \rangle = 2D_\alpha t^\alpha$. An important property of the fractional Fokker-Planck equation is that in the long time limit Boltzmann equilibrium is obtained [32]

$$p^{\text{eq}}(x) = \frac{\exp\left[-\frac{V(x)}{T}\right]}{Z} \qquad (38)$$

provided that the force is binding. Recently numerical methods which give the sample paths of the fractional Fokker-Planck equation were investigated in detail [20, 34, 35, 36, 37]. Such paths or the corresponding CTRW trajectories yield non ergodic behaviors [14]. For example in [16] the Lamperti PDF Eq. (23) of the occupation fraction was obtained from the fractional equation (37). However so far distributions of time averages of physical observables were not considered in detail.

We investigate the time average of the observable $\mathcal{O} = x$ with $-\infty < x < \infty$ so we are dealing with a continuum situation. Taking the continuum limit of Eq. (13) we find

$$f_\alpha(\overline{x}) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \text{Im} \frac{\int_{-\infty}^{\infty} dx p^{\text{eq}}(x)(\overline{x} - x + i\epsilon)^{\alpha-1}}{\int_{-\infty}^{\infty} dx p^{\text{eq}}(x)(\overline{x} - x + i\epsilon)^\alpha} \quad (39)$$

which for $0 < \alpha < 1$ is rewritten as

$$f_\alpha(\overline{x}) =$$

$$\frac{\sin \pi\alpha}{\pi} \frac{I_{\alpha-1}^<(\overline{x}) I_\alpha^>(\overline{x}) + I_{\alpha-1}^>(\overline{x}) I_\alpha^<(\overline{x})}{[I_\alpha^>(\overline{x})]^2 + [I_\alpha^<(\overline{x})]^2 + 2\cos \pi\alpha I_\alpha^>(\overline{x}) I_\alpha^<(\overline{x})}, \tag{40}$$

where

$$I_\alpha^<(\overline{x}) = \int_{\overline{x}}^{\infty} dx p^{\text{eq}}(x)|x - \overline{x}|^\alpha \qquad (41)$$

and

$$I_\alpha^>(\overline{x}) = \int_{-\infty}^{\overline{x}} dx p^{\text{eq}}(x)|\overline{x} - x|^\alpha \qquad (42)$$

and similarly for $I_{\alpha-1}^<(\overline{x})$ and $I_{\alpha-1}^>(\overline{x})$. When $\alpha \to 0$ we have $\lim_{\alpha \to 0} f_\alpha(\overline{x}) = p^{\text{eq}}(\overline{x})$ which is the continuum limit of Eq. (21). In the ergodic limit $\alpha \to 1$ we find $f_1(\overline{x}) = \delta(\overline{x} - \langle x \rangle)$.

A. Free particle.

As an example consider a particle in a domain $-l/2 < x < l/2$ undergoing an unbiased fractional random walk with reflecting walls. This is a free particle in the sense that no external field is acting on it. The time average of the particle's position $\overline{x}$ is considered, and obviously for this case $p^{\text{eq}}(x) = 1/l$ for $-l/2 < x < l/2$. Using Eq. (40) we find the PDF of $\overline{x}$

$$f_\alpha(\overline{x}) =$$

$$\frac{1}{l} \frac{N_\alpha \left(\frac{1}{4} - \frac{\overline{x}^2}{l^2}\right)^\alpha}{\left|\frac{1}{2} - \frac{\overline{x}}{l}\right|^{2(1+\alpha)} + \left|\frac{1}{2} + \frac{\overline{x}}{l}\right|^{2(1+\alpha)} + 2\left|\frac{1}{4} - \left(\frac{\overline{x}}{l}\right)^2\right|^{1+\alpha} \cos \pi\alpha}, \tag{43}$$

where $N_\alpha = (1 + \alpha)\sin \pi\alpha/(\pi\alpha)$. When $\alpha \to 1$ we have ergodic behavior $f_\alpha(\overline{x}) = \delta(\overline{x})$ since $\langle x \rangle = 0$ while in the opposite limit $f_{\alpha \to 0}(\overline{x}) = 1/l$ for $|\overline{x}| < l/2$ which is the uniform distribution, reflecting the mentioned localization of the particle in space when $\alpha \to 0$.

B. Harmonic Oscillator

We consider the time average $\overline{x}$ of a particle in a Harmonic force field $V(x)/T = x^2$ so that $p^{\text{eq}}(x) = \exp(-x^2)/\sqrt{\pi}$ and $\langle x \rangle = 0$. Using Mathematica the integrals Eqs. (41,42) can be calculated explicitly and expressed in terms of tabulated confluent Hypergeometric functions. In Fig. 1 the PDF of $\overline{x}$ Eq. (40) is presented, and a transition from a narrow distribution when $\alpha \to 1$ to a Gaussian distribution when $\alpha \to 0$, $\lim_{\alpha \to 0} f_\alpha(\overline{x}) = p^{\text{eq}}(\overline{x})$ is found. Using Eq. (40) it is easy to show that $\langle \overline{x} \rangle = 0$, $\langle \overline{x}^2 \rangle = (1 - \alpha)\langle x^2 \rangle$ with $\langle x^2 \rangle = 1/2$ for $p^{\text{eq}}(x)$ under consideration, and $\langle \overline{x}^4 \rangle = (1 - \alpha)(3 - 2\alpha)\langle x^2 \rangle^2$. Only when $\alpha \to 0$ we have Gaussian statistics with $\langle \overline{x}^4 \rangle = 3\langle \overline{x}^2 \rangle^2$. The PDF $f_\alpha(\overline{x})$ at its maximum on $\overline{x} = 0$ is

$$f_\alpha(\overline{x} = 0) = \frac{\Gamma(\frac{\alpha}{2})\tan(\frac{\pi\alpha}{2})}{\Gamma(\frac{1+\alpha}{2})\pi}, \qquad (44)$$
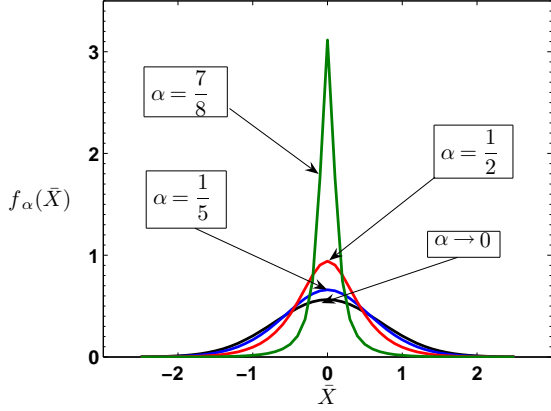
FIG. 1: The PDF of $\overline{x}$ for a particle in a Harmonic force field Eq. (40). We find a transition between an ergodic behavior: a delta distribution of $\overline{x}$ when $\alpha \to 1$, to the localization limit where the distribution of $\overline{x}$ is Gaussian when $\alpha \to 0$.

which is equal to $p^{\text{eq}}(x = 0) = 1/\sqrt{\pi}$ when $\alpha \to 0$ and diverges when $\alpha \to 1$ as expected from an ergodic behavior. For the Harmonic oscillator and the Free particles the maximum of $f_\alpha(\overline{x})$ is found on the ensemble average $\langle x \rangle = 0$, so the most likely result for $\overline{x}$ is $\langle x \rangle$. In the next subsection we consider a case where a minimum of $f_\alpha(\overline{x})$ is found on the ensemble average.

C. Double well potential.

An interesting case is the symmetric double well potential $V(x)/T = (x^4/4 - x^2/2)/T$ so $\langle x \rangle = 0$. When $T \to 0$, $p^{\text{eq}}(x)$ has two peaks centered on the two local minima of the double well potential. In this low temperature case and in the limit $\alpha \to 0$ we expect to find the particle either in the left well or in the right well for a time scale comparable to the measurement time. Hence when $T \to 0$ and $\alpha \to 0$ the PDF of the time average $\overline{x}$, $f_\alpha(\overline{x})$ is a sum of two delta functions since either $\overline{x} = 1$ or $\overline{x} = -1$. When $\alpha \to 1$ we expect an ergodic behavior, and then PDF $f_1(\overline{x}) = \delta(\overline{x})$, since $\langle x \rangle = 0$. So for low temperatures we expect a transition in the behavior of $f_\alpha(\overline{x})$ from a bimodal shape when $\alpha \to 0$ to a PDF with a single peak centered on zero when $\alpha \to 1$. Hence we will have a critical value α_c. For $\alpha < \alpha_c$ the shape of $f_\alpha(\overline{x})$ is bimodal with a minimum on $\overline{x} = 0$, while for $\alpha > \alpha_c$ a maximum on $\overline{x} = 0$ is found. These low temperature behaviors are shown in Fig. 2. For high temperatures (compared with the barrier height) the bimodal solution of $p^{\text{eq}}(x)$ turns into a flatter shape. Since $\lim_{\alpha \to 0} f_\alpha(\overline{x}) = p^{\text{eq}}(\overline{x})$ we will not observe the bimodal shape of $\lim_{\alpha \to 0} f_\alpha(\overline{x})$ when $T \to \infty$. Such high temperature behavior is shown in Fig. 3.

Investigating the extremum of $p^{\text{eq}}(x)$ on $x = 0$ it is easy to show that α_c is finite for any finite temperature

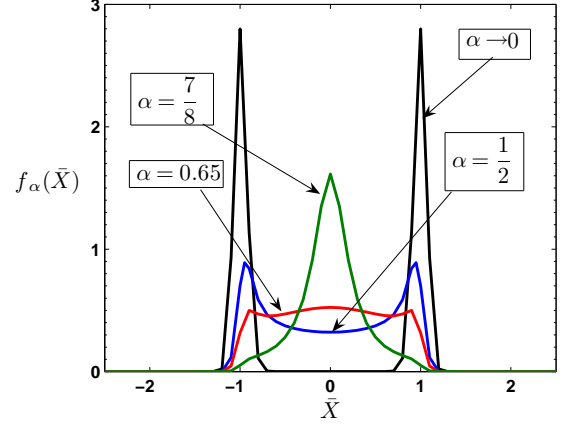FIG. 2: The PDF of $\overline{x}$ for a particle in the double well potential with $T = 0.01$. A transition between a bimodal behavior when $\alpha < \alpha_c$ to a PDF with a peak on $\overline{x} = 0$ when $\alpha > \alpha_c$ is observed ($\alpha_c \simeq 0.59$ for this case). In the ergodic limit $\alpha \to 1$ $f_\alpha(\overline{x})$ is a delta function centered on the ensemble average $\langle x \rangle = 0$. In the localization limit $\alpha \to 0$ $f_\alpha(\overline{x})$ is equal to the population density $p^{\text{eq}}(\overline{x})$.

and $\alpha_c \to 0$ when $T \to \infty$. For $T = 0$ we have only two states in the system, either $x = -1$ or $x = 1$ corresponding to two minima of the double well potential. The analysis is then very similar to the two state ballistic Lévy walk model [10, 38]. Clearly $\overline{x}$ is the residence time in state $x = 1$ minus the residence time in state $x = -1$ divided by the measurement time t. Since the sum of these two residence times is the measurement time we can use the Lamperti distribution Eq. (23) to predict the distribution of $\overline{x}$. So when $T \to 0$

$$\lim_{T \to 0} f_\alpha(\overline{x}) =$$

$$\frac{2 \sin \pi \alpha}{\pi} \frac{\left(1 - \overline{x}^2\right)^{\alpha - 1}}{\left(1 + \overline{x}\right)^{2\alpha} + \left(1 - \overline{x}\right)^{2\alpha} + 2\left(1 - \overline{x}^2\right)^\alpha \cos \pi \alpha} \tag{45}$$

which was found already in [26, 39]. We find that $\alpha_c = 0.59461 \cdots$ when $T \to 0$. The behavior of α_c versus temperature is shown in Fig. 4 and the transition between the low and high temperature cases is presented.

D. Possible Physical Applications

It is interesting to verify in experiments our theoretical predictions and here we discuss three examples. Generally systems with CTRW type of dynamics are natural candidates for the investigation of weak ergodicity breaking, provided that information of single particle dynamics can be recorded.

Sub-diffusion $\langle x^2 \rangle \sim t^\alpha$ *of a bead in a polymer network* was measured by Wong et al [40]. The measured [40]
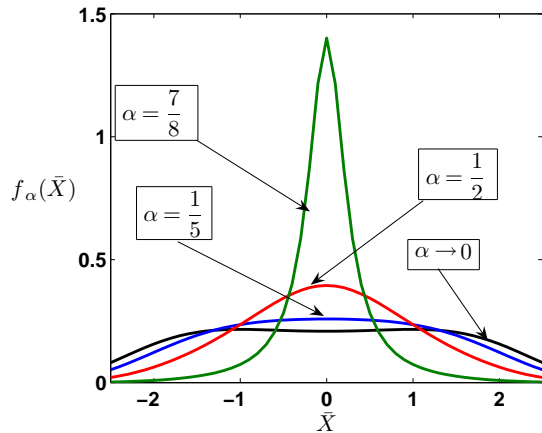
FIG. 3: The same as Fig. (2) however now $T = 7$. The bimodal shape presented in Fig. (2) is smoothed and we barely observe bi-modal behavior, since the equilibrium density $p^{\mathrm{eq}}(x)$ is not centered around the two minima of the double well potential, when the temperature is high.

FIG. 4: The critical exponent α_c versus temperature for a particle in a double well potential. α_c marks the transition between a local minimum to a local maximum of the PDF of $\overline{x}$ on $\overline{x} = 0$. When $T \to \infty$ $\alpha_c \to 0$ since in this limit and when $\alpha \to 0$ $f_\alpha(\overline{x})$ is equal to the population density $p^{\mathrm{eq}}(\overline{x})$ which does not "feel" the wells when the temperature is high (single peak). When $T \to 0$ we have $\alpha_c \simeq 0.595$.

exponent α depends on the ratio of the size of the bead and the linear size of the mesh of the network l (roughly a μm). We suggest to add an external binding field, for example an harmonic trap. The time averages of a single particle coordinate can then be measured, and according to our theory its distribution is given by Eq. (13). Such measurement can provide insight into the nature of disorder, for example is it quenched or annealed [22].

Messenger RNA molecules inside live E. coli cells exhibit anomalous diffusion $\langle x^2 \rangle \sim t^\alpha$ and $\alpha = 3/4$ [41]. Due to the finite size of the cell the motion is bounded. It would be interesting to investigate time averages of the position of the single molecule, or occupation time statistics, to investigate deviations from ergodicity. Our theory gives a prediction for the distribution of these observables, which can be tested in experiment.

Blinking quantum dots exhibit ergodicity breaking which is already measured in experiments [9, 11, 12]. So far a simple two state picture of the quantum dots was used, either the dot is on and it emits many photon, or it is off [10]. Then ergodicity breaking of the time averaged fluorescence intensity is similar to the time average of a particle in the double well potential in the limit of $T \to 0$, in the latter case either the particle is the left well or in the right well. More careful analysis reveals that some dots deviate from a simple two state process [12]. Then our more general theory can be used in principle to predict distribution of time averaged intensity beyond the existing two state approach.
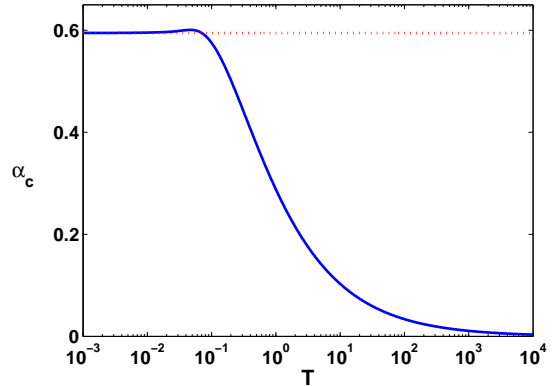
V. FROM CONTINUOUS TIME RANDOM WALK TO WEAK ERGODICITY BREAKING

In this Sec. we derive our main results using the CTRW approach. To reach Eq. (13) we assumed among other things that: (i) the PDF of the occupation time t_i is the one sided Lévy PDF Eq. (3) and (ii) that the total measurement time $t = \sum_{i=1}^{L} t_i$ is a random variable, while in Physical experiments the measurement time is fixed. These assumptions are relaxed now using two types of CTRW models. Thermal CTRW describe a Physical situation where the particle is undergoing the random walk in contact with a thermal heat bath. In this case the equilibrium distribution of an ensemble of particles is Boltzmann's distribution. The second case describes a system far from thermal equilibrium, where a non-thermal equilibrium is reached.

We consider a renewal process for a system with L states $i = 1, ..., L$. The system starts in state i, it waits in this state until time $\bar{t}_1$, it then jumps to some other state say state l, it waits in state l until time $\bar{t}_2$ and then makes another jump. The sojourn times between jump events τ are independent identically distributed random variables with a common PDF $\psi(\tau)$. Our focus is on the case where $\psi(\tau)$ has a long tail $\psi(\tau) \propto \tau^{-(1+\alpha)}$ when $\tau \to \infty$ so $\langle \tau \rangle = \infty$ when $0 < \alpha < 1$. After waiting in a state i a transition to state $j \neq i$ takes place, with probability w_{ji} ($0 \leq w_{ji} \leq 1$, $\sum_{j=1}^{L} w_{ji} = 1$ and $w_{ii} = 0$). We assume that transition probabilities w_{ji} are such that in the limit of long measurement times all states are visited what ever is the initial condition. In other words the system is not decomposable into non-accessible regions in the space it samples, where once the system starts in a certain region it cannot explore all other states. Such

a case corresponds to strong ergodicity breaking.

Let N be the random number of jump events (renewals) in the time interval $(0, t)$. Dots on the time axis on which jumps from one state to another happen are denoted with $\bar{t}_i$ and clearly $\bar{t}_N < t < \bar{t}_{N+1}$. Let n_i be the number of transitions out of state i and clearly $N = \sum_{i=1}^{L} n_i$. Let τ_l^i be the l th sojourn time in state i. And let k be the state of the system at time t. A schematic presentation of the process with three states is shown in Fig. 5. Statistics of the number of renewals N in $(0, t)$ is a well investigated problem [24, 26, 42] for example $\langle N \rangle \sim t^\alpha$.

For the CTRW on a one dimensional lattice the states $i = 1, ...L$ correspond to the position of the particle on a finite lattice. Then for example the time average of the coordinate of the particle is $\overline{x} = \sum_{i=1}^{L} it_i/t$ where t_i is the occupation time in state i (see Fig. 5). However our considerations are more general. For example for blinking quantum dots [9, 10, 11, 12] one state (say $i = 1$) may denote an on state in which many photons are emitted and state $i = 2$ is the off state. This system is non-thermal since it is driven by a strong laser field. On the other hand the CTRW dynamics of a probe bead immersed in a polymer actin network [40] is an example for a thermal CTRW motion in a system with a well defined temperature T.

A specific example is the CTRW on a lattice with jumps to nearest neighbors only. A particle on i has a probability of jumping left q_i and a probability of jumping right $1 - q_i$ so

$$w_{i-1,i} = q_i \quad \text{and} \quad w_{i+1,i} = 1 - q_i. \tag{46}$$

Reflecting boundary conditions $q_L = 1$ and $q_1 = 0$ are assumed. For $i \neq 1, L$ we must have $q_i \neq 0$ and $q_i \neq 1$ so that all lattice points be visited. Between jumps the particle waits on a lattice point. The waiting times between the jumps are independent, identically distributed random variables with a common PDF $\psi(\tau)$. This type of random walk leads to anomalous subdiffusion $\langle x^2 \rangle \sim t^\alpha$ when $q_i = 1/2$ and the system is infinite [2, 42].

The ratio $v_i = n_i/N$ is called the visitation fraction. The population fraction p_i^{eq} is found by considering the ensemble of M non interacting systems. Letting these systems evolve from some initial condition and waiting for the long time limit, $\lim_{M \to \infty} M_i/M = p_i^{\text{eq}}$ where M_i is the number of systems in state i. The population fraction is determined from $w \cdot p^{\text{eq}} = p^{\text{eq}}$.

After many jumps $N \to \infty$ and for any initial condition the visitation fraction reaches an equilibrium and

$$p_i^{\text{eq}} = \lim_{N \to \infty} v_i = v_i^{\text{eq}} \tag{47}$$

so $w \cdot v = v$. To see this note that the visitation fraction is given by $v_i = \sum_{n=1}^{N} \theta_i(n)/N$, where n is a counter of the number of jumps, and $\theta_i(n) = 1$ if the particle is on i after n steps, otherwise it is zero. In the long time limit the PDF of v_i will converge to a narrow distribution centered around its mean so $v_i \simeq \sum_{n=1}^{N} \langle \theta_i(n) \rangle/N$. Let

$p_i(n)$ be the probability to be on i after n steps. By definition $\theta_i(n) = 1$ with probability $p_i(n)$ and $\theta_i(n) = 0$ with probability $1 - p_i(n)$. Hence

$$v_i \simeq \frac{\sum_{n=1}^{N} p_i(n)}{N} \tag{48}$$

or in vector notation $v = (v_1, \cdots, v_L)$, $p(n) = (\cdots, p_i(n) \cdots)$ we have $v \simeq \sum_{n=1}^{N} p(n)/N$. This means that ergodicity holds in discrete time, where the operational time is the number of steps, not the real time. Hence the term *weak* ergodicity breaking [7] is very appealing. Multiplying Eq. (48) with w from the left and using $p(n+1) = wp(n)$ we have $w \cdot v \simeq \sum_{n=1}^{N} p(n+1)/N$. Hence when $N \to \infty$ we have $w \cdot v = v$ which holds in the long time limit. It is important to realize that the visitation fraction and the population fraction are equal since all sojourn times have a common distribution $\psi(\tau)$. We will later consider the more general case where different states may have different waiting times PDFs.

For the one dimensional CTRW on a lattice the equilibrium population and hence the visitation fraction is determined from Eq. (46)

$$p_i^{\text{eq}} = q_{i+1} p_{i+1}^{\text{eq}} + (1 - q_{i-1}) p_{i-1}^{\text{eq}}. \tag{49}$$

Using reflecting boundary conditions and Eq. (49)

$$p_i^{\text{eq}} = \lim_{N \to \infty} v_i = \frac{1}{1 - q_i} \Pi_{k=2}^{i} \frac{1 - q_k}{q_k} p_1^{\text{eq}} \tag{50}$$

and from normalization

$$p_1^{\text{eq}} = v_1^{\text{eq}} = \left[1 + \sum_{i=2}^{L} \frac{1}{1 - q_i} \Pi_{k=2}^{i} \frac{1 - q_i}{q_i} \right]^{-1}. \tag{51}$$

When the particle undergoing the CTRW process is coupled to a thermal heat bath, we apply usual detailed balance condition on the transition probabilities [15]. In this case the visitation fraction will be described by Boltzmann statistics. For example if q_i is a constant $q > 1/2$ the random walk is biased, which Physically corresponds to an external force field $F < 0$ driving the particles to the left. Using lattice spacing a and letting the system be semi-infinite $L \to \infty$, thermal detailed balance condition gives the ratio between the probability of jumping left from point i and the probability of jumping right from point $i - 1$

$$\frac{q_i}{1 - q_{i-1}} = \frac{q}{1 - q} = \exp(\frac{|F|a}{T}). \tag{52}$$

Using Eqs. (47,50,51,52) Boltzmann's statistics holds both for the visitation and the population fractions

$$\lim_{N \to \infty} v_i = p_i^{\text{eq}} = \frac{\exp\left(-\frac{E_i}{T}\right)}{Z} \tag{53}$$

for $i > 1$ where $E_i = |F|ai$ is the potential energy, Z is a normalization and for the reflecting boundary $p_1^{\text{eq}} =$

Time line

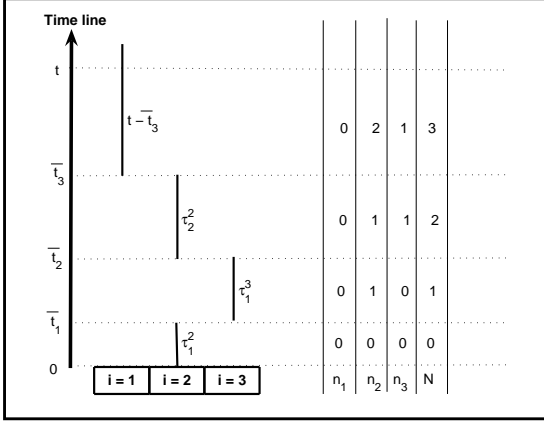|	0	2	1	3
	0	1	1	2
	0	1	0	1
	0	0	0	0
	n_1	n_2	n_3	N

i = 1 | i = 2 | i = 3

FIG. 5: A schematic diagram of the process for a system with three states, starting in state 2 and ending in state $k = 1$. In this example the occupation times are $t_1 = t - \bar{t}_3$, $t_2 = (\bar{t}_1 - 0) + (\bar{t}_3 - \bar{t}_2) = \tau_1^2 + \tau_2^2$ and $t_3 = \bar{t}_2 - \bar{t}_1 = \tau_1^3$.

$[1 - \exp(-|F|a/T)]/2$. More general thermal detailed balance conditions [15] show that Eq. (53) is valid for binding force fields and not limited to the case F being a constant.

The time average of a physical observable is as before

$$\overline{\mathcal{O}} = \frac{\sum_{i=1}^{L} \mathcal{O}_i t_i}{t}, \qquad (54)$$

where now the measurement time t is fixed and $\sum_{i=1}^{L} t_i = $

t. Let $\vec{\mathcal{O}} = \{\mathcal{O}_1, \cdots \mathcal{O}_L\}$. We consider the moment generating function,

$$\hat{f}_{t,\vec{\mathcal{O}}}(u) = \langle \exp\left(-u \sum_{i=1}^{L} \mathcal{O}_i t_i\right) \rangle, \qquad (55)$$

and in double Laplace space

$$\hat{f}_{s,\vec{\mathcal{O}}}(u) = \int_0^\infty e^{-st} \langle \exp\left(-u \sum_{i=1}^{L} \mathcal{O}_i t_i\right) \rangle \mathrm{d}t \qquad (56)$$

so s, t and $u, \sum_{i=1}^{L} \mathcal{O}_i t_i$ are two Laplace pairs. Let $\vec{n} = \{n_1, \cdots, n_L\}$. We consider the generating function conditioned that the system made N transitions and $\vec{n}$ describes the number of renewals in each state. The occupation time in state $i \neq k$ is

$$t_i = \sum_{l=1}^{n_i} \tau_l^i \qquad (57)$$

and for state k

$$t_k = t - \bar{t}_N + \sum_{l=1}^{n_k} \tau_l^k. \qquad (58)$$

The time $t - \bar{t}_N$ is called the backward recurrence time, it is the time between the last jump event in $(0, t)$ and the measurement time t. Using Eqs. (57,58) the conditioned generating function is

$$\hat{f}_{s,\vec{\mathcal{O}},N,\vec{n}}(u) = \langle \int_0^\infty \mathrm{d}t \exp\left[-st - u\mathcal{O}_k\left(t - \bar{t}_N + \sum_{l=1}^{n_k} \tau_l^k\right) - \sum_{i=1, i\neq k}^{L} u\mathcal{O}_i \sum_{l=1}^{n_i} \tau_l^i \right] I\left(\bar{t}_N < t < \bar{t}_{N+1}\right) \rangle \qquad (59)$$

where $I(x) = 1$ if the condition in the parenthesis is true, other wise $I(x) = 0$. First we integrate over t and obtain

$$\hat{f}_{s,\vec{\mathcal{O}},N,\vec{n}}(u) = \langle \frac{e^{-s\bar{t}_N} - e^{-s\bar{t}_{N+1} - u\mathcal{O}_k(\bar{t}_{N+1} - \bar{t}_N)}}{s + u\mathcal{O}_k} e^{-\sum_{i=1}^{L} u\mathcal{O}_i \sum_{l=1}^{n_i} \tau_l^i} \rangle, \qquad (60)$$

then we use the assumption of independent and identically distributed sojourn times τ, and the identities $\bar{t}_N = \sum_{i=1}^{L} \sum_{l=1}^{n_i} \tau_l^i$, $\bar{t}_{N+1} = \bar{t}_N + \tau_k^{n_k+1}$ to find

$$\hat{f}_{s,\vec{\mathcal{O}},N,\vec{n}}(u) = \frac{\Pi_{i=1}^{L} \hat{\psi}^{n_i}(s + u\mathcal{O}_i)\left[1 - \hat{\psi}(s + u\mathcal{O}_k)\right]}{s + u\mathcal{O}_k}, \qquad (61)$$

where $\hat{\psi}(s) = \int_0^\infty \psi(\tau) \exp(-s\tau) \mathrm{d}\tau$ is the Laplace transform of $\psi(\tau)$.

In the limit of long measurement time, corresponding to the usual small s and u limit, their ratio being finite,

the system will reach an equilibrium for the number of renewals in each state. Namely from Eq. (47) the visitation fraction will satisfy

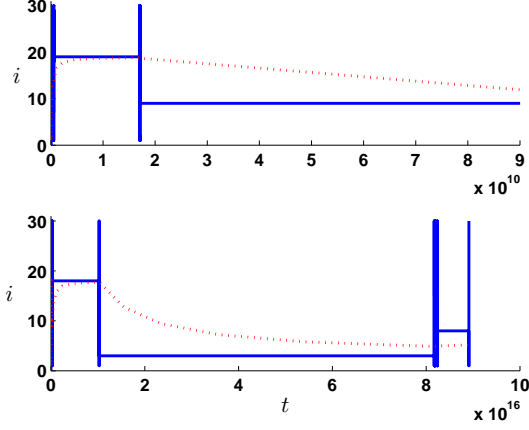$$v_i = \lim_{N \to \infty} \frac{n_i}{N} = p_i^{\mathrm{eq}}. \qquad (62)$$

FIG. 6: Trajectory of a single CTRW particle on a lattice, with $\alpha = 0.3$ (solid curve, blue online). Long waiting times, of the order of the measurement time, dominate the landscape. The time average $\overline{x}$ is a random variable (dotted red curve).

We use Eq. (62) in Eq. (61), then insert the usual small s behavior [5, 24, 26, 42]

$$\hat{\psi}(s) \sim 1 - As^\alpha \qquad (63)$$

which corresponds to $\psi(\tau) \sim A\tau^{-(1+\alpha)}/|\Gamma(-\alpha)|$ and find

$$\hat{f}_{s,\vec{\mathcal{O}},k}(u) \sim \frac{(s + u\mathcal{O}_k)^{\alpha-1}}{\sum_{i=1}^L p_i^{\text{eq}}(s + u\mathcal{O}_i)^\alpha}. \qquad (64)$$

Summing over all final states k, with the final weights, we find

$$\hat{f}_{s,\vec{\mathcal{O}}}(u) \sim \frac{\sum_{i=1}^L p_i^{\text{eq}}(s + u\mathcal{O}_i)^{\alpha-1}}{\sum_{i=1}^L p_i^{\text{eq}}(s + u\mathcal{O}_i)^\alpha}. \qquad (65)$$

Using a method found in the Appendix of Ref. [26] we invert Eq. (65) and find our main Eq. (13).

A. Numerical Examples

To demonstrate our results we consider an unbiased CTRW. We consider a model with $L = 30$ sites on $i = 1, ...30$ jumps are to nearest neighbors only with $q_i = 1/2$ with periodic boundary conditions. We used the waiting time PDF $\psi(\tau) = \alpha\tau^{-\alpha-1}$ for $\tau > 1$ otherwize $\psi(\tau) = 0$. Simulating trajectories of a single particle we calculate the time average $\overline{x}$ and then repeat the experiment many times and construct the distribution of $\overline{x}$.

In Figs. 6,7 we show single particle trajectories and their time average for $\alpha = 0.3$ and $\alpha = 0.75$ respectively. The time average is clearly a fluctuating random variable, due to long sticking times in states of the system. Notice that the particle visits all lattice points, and the phase space is not decomposable into inaccessible regions as
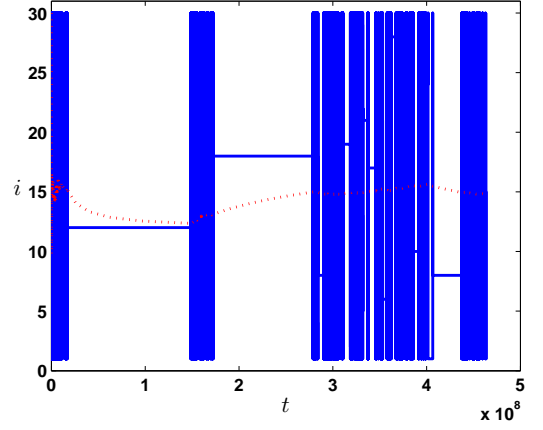

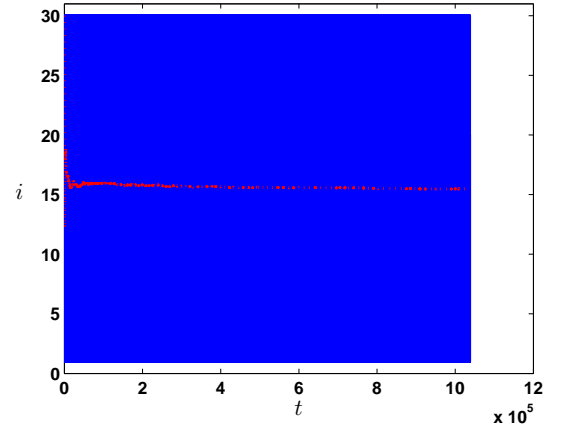FIG. 7: Same type of non-ergodic behavior as found in Fig. 6 however now $\alpha = 0.75$.

FIG. 8: Same as Fig. 6 however now $\psi(\tau) = 5\tau^{-6}$ for $\tau > 1$ so $\alpha = 5$. After a short transient the time average converges to the ensemble average on 15.5 indicating ergodicity.

found for strong ergodicity breaking. For a waiting time PDF with $\alpha = 5$, we have a finite average waiting time, and hence as shown in Fig. 8 we find an ergodic behavior $\overline{x} \simeq \langle x \rangle = (L + 1)/2 = 15.5$ in the long time limit.

In Figs. 9,10 we present the PDF of $\overline{x}$ for $\alpha = 0.75$ and $\alpha = 0.3$ respectively. Comparison between simulations and theory Eq. (13) show excellent agreement without fitting. In Eq. (13) we use $p_i^{\text{eq}} = 1/L$ which is the obvious population probability. The number of realizations was 120000 and the simulation time $t = 10^8, 10^{12}$ for Figs. 9,10 respectively. In Figs. 9,10 we also show the continuum approximation Eq. (43). From Figs. 9,10 we see that the structure of the lattice is encoded in the distribution of the time average $\overline{x}$. Since the observable at any given moment of time attains the values $x = 1, ...30$ we have 30 divergences in Figs. 9,10 in agreement with the more general rule discussed under Eq. (16). When
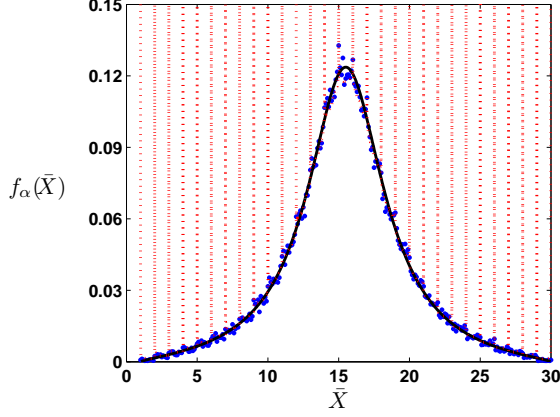
FIG. 9: Distribution of the time average $\overline{x}$ for $\alpha = 3/4$. Numerical simulations of the CTRW process on a lattice (dots) are well approximated with the continuum limit Eq. (43) (solid curve). The dotted curve with divergences on the lattice points is the analytical theory Eq. (13).
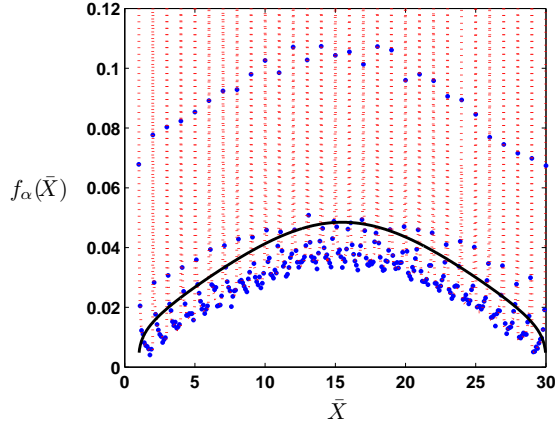

FIG. 10: Same as Fig. 9 for $\alpha = 0.3$. Now the fluctuations are larger compared with the $\alpha = 3/4$ case and the underlying structure of the lattice is important. Ofcourse bin size must be made small enough for the lattice effect to be observed.

the system is made large these effects become negligible and the continuum approximation works well.

B. Non identical waiting time distributions

The CTRW considers a situation where a single waiting time PDF $\psi(\tau)$ describes the dynamics. What happens when the waiting times in the states i are not identically distributed? For example consider the mentioned blinking quantum dots [9, 10, 11, 12]. The quantum dot when interacting with a laser field will switch between an on state $(+)$ where many photons are emitted and an

off $(-)$ state. The sojourn times in state on (and off) are independent identically distributed random variables [43]. The PDF of sojourn times in states on and off follow power law statistics atleast within a long experiment time [12] and in Laplace space $\hat{\psi}_{\pm}(s) \sim 1 - A_{\pm}s^{\alpha} + \cdots$. This two state renewal process is characterized with two amplitudes A_+ and A_- and in this sense it differs from the usual CTRW. It is worthwhile noting that the visitation fraction in states $\pm$ clearly satisfy

$$\lim_{N \to \infty} v_{\pm} = \lim_{N \to \infty} \frac{n_+}{N} = \lim_{N \to \infty} \frac{n_-}{N} = \frac{1}{2} \qquad (66)$$

in the limit of long measurement time, where N is the total number of transitions between states on and off. If we consider an ensemble of M independent blinking dots the population fraction of the number of dots in state on $(+)$ M_+ and off $(-)$ M_- is

$$p_{\pm}^{eq} = \lim_{M \to \infty} \frac{M_{\pm}}{M} = \frac{A_{\pm}}{A_- + A_+}, \qquad (67)$$

where the population fraction is measured in the limit of long measurement time. So here the visitation fraction and the population fraction are non-identical if $A_+ \neq A_-$.

More generally we consider the renewal dynamics with power law waiting times in each state however now

$$\hat{\psi}_i(s) \sim 1 - A_i s^{\alpha} \qquad (68)$$

when the Laplace variable $s \to 0$, $A_i > 0$ for $i = 1, \cdots, L$ and $0 < \alpha < 1$. In this case the population fractions are related to the visitation fractions according to

$$p_i^{\text{eq}} = \lim_{N \to \infty} \frac{A_i v_i}{\sum_{i=1}^{L} A_i v_i} \qquad (69)$$

and $w \cdot v = v$. Now the main Eqs. derived in this Sec. must be modified, for example Eq. (61)

$$\hat{f}_{s,\vec{\mathcal{O}},N,\vec{n}}(u) = \frac{\Pi_{i=1}^{L} \hat{\psi}_i^{n_i}(s + u\mathcal{O}_i)\left[1 - \hat{\psi}_i(s + u\mathcal{O}_k)\right]}{s + u\mathcal{O}_k}. \qquad (70)$$

Then using Eqs. (68,69,70) we find Eq. (13) (the method is nearly identical to the case where all the waiting times are identical). Thus while the dynamics clearly differs from the usual CTRW with a single waiting time PDF, and the visitation fraction is not identical to the population fraction, our main Eq. for the distribution of the time averages Eq. (13) is still valid.

Another situation is when the system has different types of waiting times, for example some states may have exponential waiting times while others follow power law statistics. Or we may have some states with a power law waiting time PDF with an exponent $0 < \alpha_1 < 1$ and for other states an exponent $0 < \alpha_2 < \alpha_1$. Also in this case our main result Eq. (13) will be valid. In the long time limit the system will occupy only the states with

the smallest $\alpha < 1$. Only those states are relevant for the calculation of the distribution of time averages Eq. (13). Other states might be visited many times so their visitation fraction is not necessarily small, still the time the system spends in these states is short and they do not contribute to the time average.

VI. DISCUSSION

To summarize we have obtained very general distributions of time averages of physical observables of weakly non-ergodic systems Eqs. (13,39). Unlike usual ergodic statistical mechanics where the time averages are equal to the ensemble averages, we find large fluctuations of time averages. Unlike strong ergodicity breaking, the space is not separated into inaccessible regions. Instead the system explores all states and the number of visits per state i n_i is large. However due to the power law sojourn times the dynamics is non-stationary and non-ergodic. Since exploration of space is possible in weak ergodicity breaking, we were able to construct a rather general statistical theory for the distribution of time averages which is valid in the long time limit and does not depend on the initial conditions of the system. Further, the exploration of the cells $i = 1, ...L$ leads to relations between the non-ergodic statistical properties of a single system, and the equilibrium populations of an ensemble of systems. Hence the distribution of time averages Eq. (13) depends on population probabilities p_i^{eq}s and when thermal detailed balance is applied these probabilities are given by Boltzmann's canonical law. Such behavior was found in two classes of models: (a) for systems with a common power law waiting time PDF $\psi(\tau)$ where the visitation fraction is equal to the population fraction and (b) for systems with different waiting times PDFs where the visitation fraction is not equal to the population fraction. In both cases the population fraction is not identical to the occupation fraction, the latter remaining a random variable when $0 < \alpha < 1$. Due to the large number of applications of the CTRW model, our theory may find its applications in several systems. The mathematical foundation of the theory is Lamperti's generalized arcsine law and Lévy's statistics, while usual type of statistical mechanics is based on the Gaussian central limit theorem. Due to the deep relations between the stochastic CTRW model and other models of anomalous diffusion, e.g. the quenched trap model and deterministic dynamics our non-ergodic theory might find more general justification.

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